SAND2001-1733P

Physics Applications in the ALEGRA Framework

1st MIT Conference on Fluid and Solid Mechanics

Daniel E. Carroll

Allen C. Robinson

Michael K. Wong

J. Randy Weatherby

Computational Physics Research and Development

Thomas A. Haill

Target and Z Pinch Theory Department

C. David Turner

EM Plasma Physics Analysis Department

Sandia National Laboratories, Albuquerque, NM, USA

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

Sandia National Laboratories

Overview

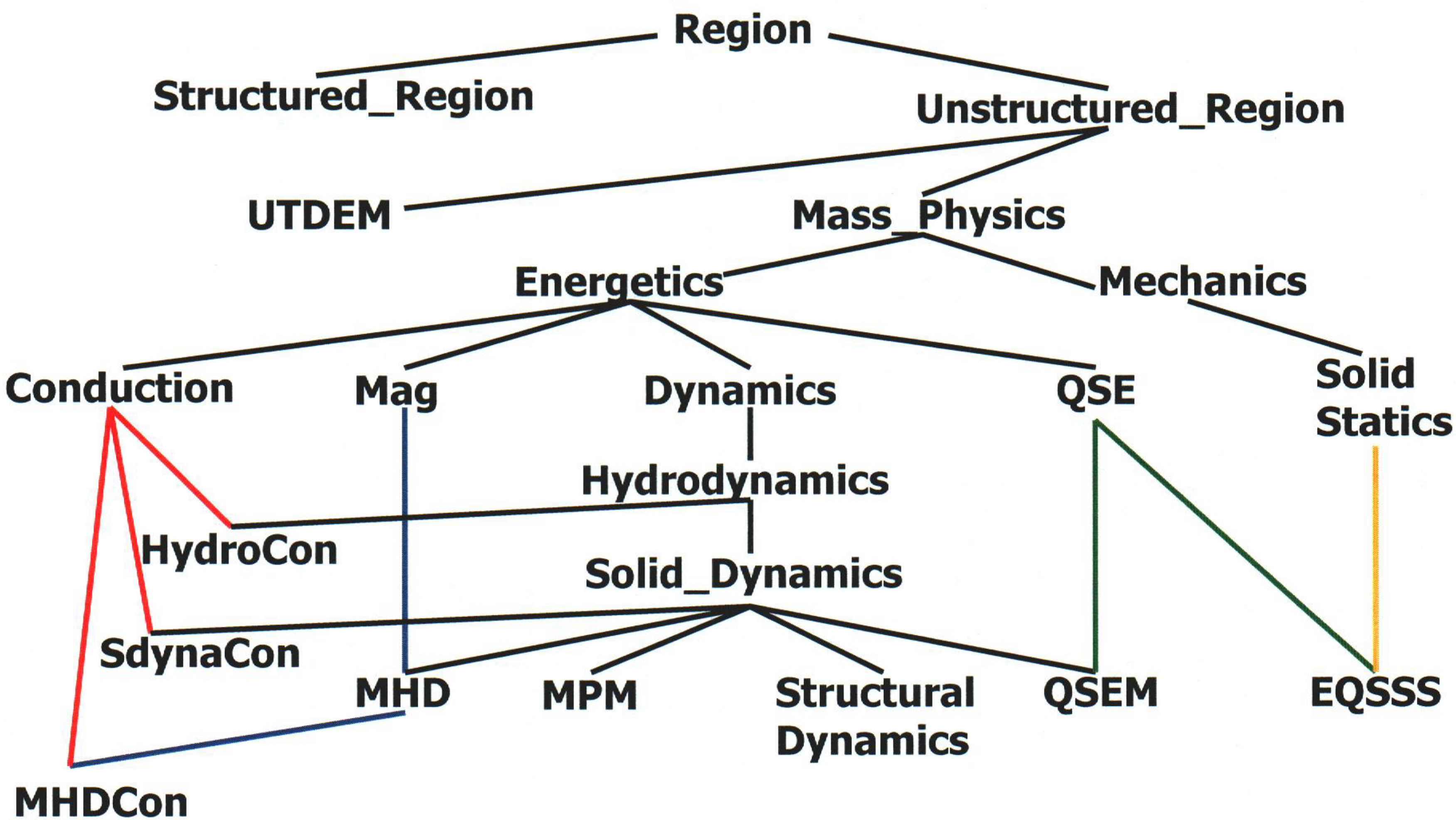
- ALEGRA Physics Framework
- Solid Dynamics and General Capabilities
  - Lagrangian-ALE-Eulerian
  - Materials
- Advanced Physics
  - Transient Electromagnetics
  - Electromechanics
    - Electro-quasistatic mechanics
    - Magnetohydrodynamics

ALEGRA Physics Framework

- ALEGRA supports a variety of physics classes
  - Basic, single physics solutions – examples:
    - Solid dynamics
    - Magnetics
    - Electrostatics
  - Coupled physics solutions - examples
    - Electromechanics
    - Magnetohydrodynamics
    - Transient electromagnetics
  - Each physics is derived from a basic, abstract physics class, containing the discretization topology.

Sandia National Laboratories

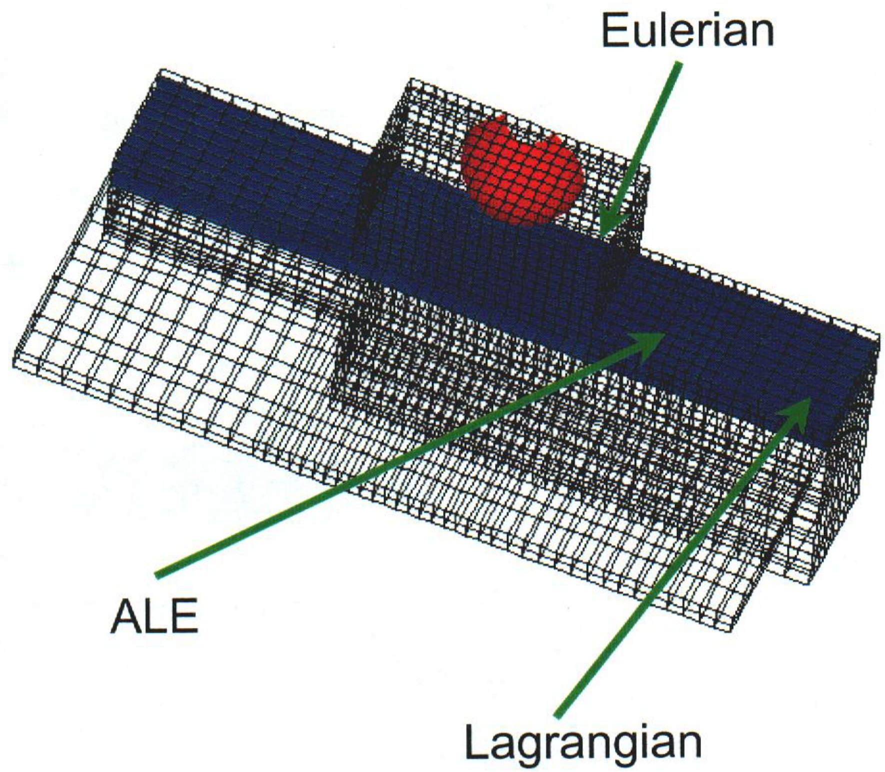
ALEGRA Physics Hierarchy (abridged)



Sandia National Laboratories

Multi-Material ALE and Solid Dynamics

- Region composed of Element Blocks
- Element Blocks may be Lagrangian, ALE, or Eulerian
- A Region may be composed of many blocks of any mesh type.
- The mesh type of blocks may be changed during calculation.
- ALE and Eulerian blocks must account for advection of material through the mesh
  - ALE mesh smoothing algorithms (Tipton)
  - 2nd order van Leer advection



Sandia National Laboratories

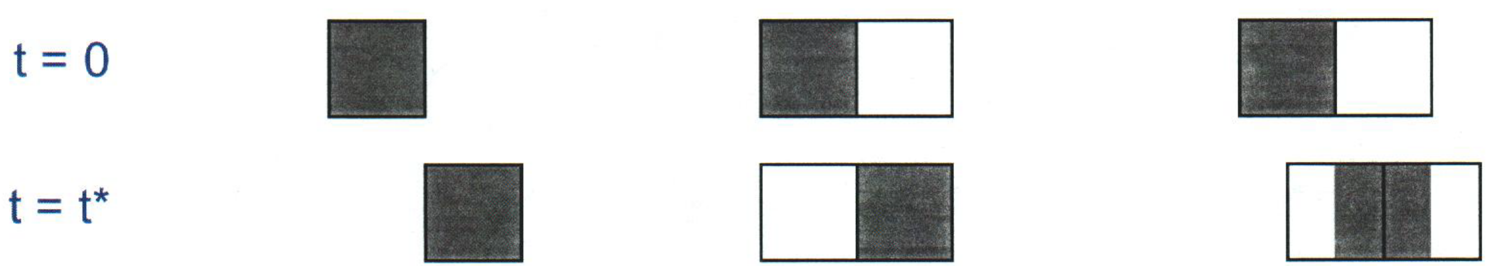
ALE Concept

Integral Form of the Conservation of Mass Equation

$$\frac{d}{dt}\int_V (\rho\, dV) + \int_s \rho(u_i - U_i) n_i ds = 0$$

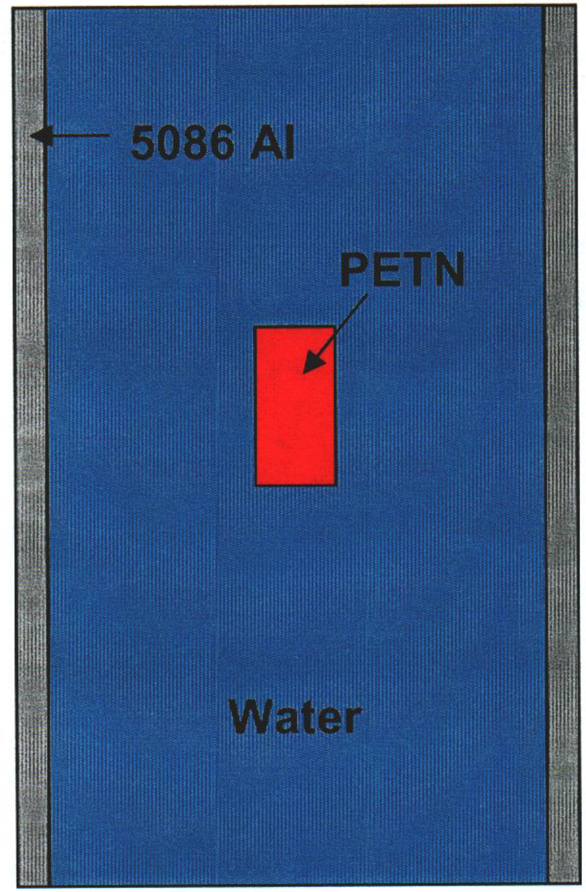
where u_i is the velocity of the fluid and U_i is the velocity of the boundary surface of the grid.

$u_i = U_i$ -> Lagrangian $U_i = 0$ -> Eulerian $u_i = U_i$ -> ALE



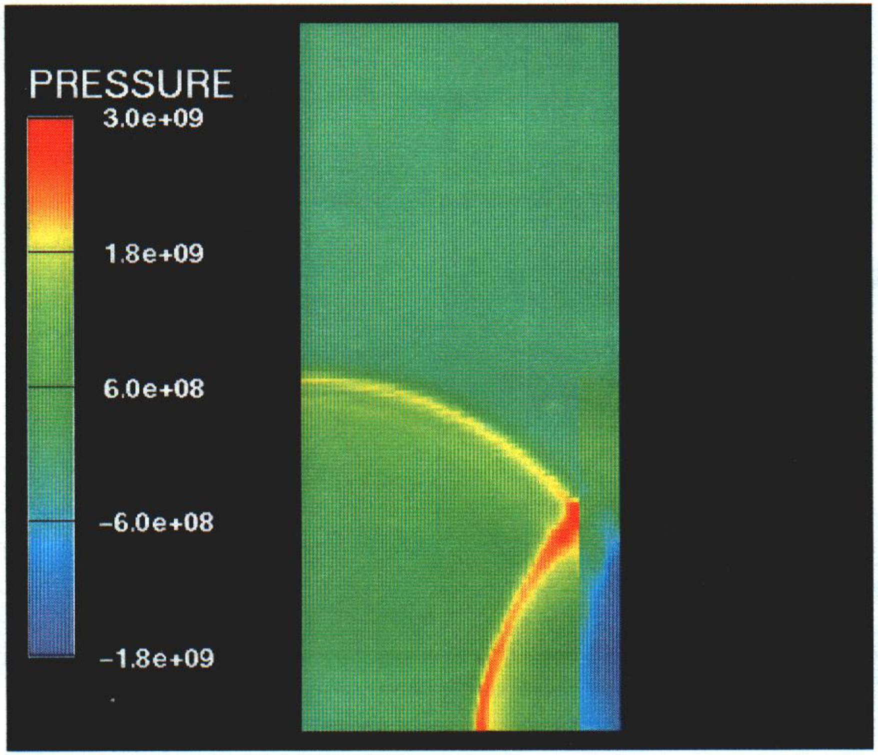
Solid Dynamics: Hydrobulge Simulations

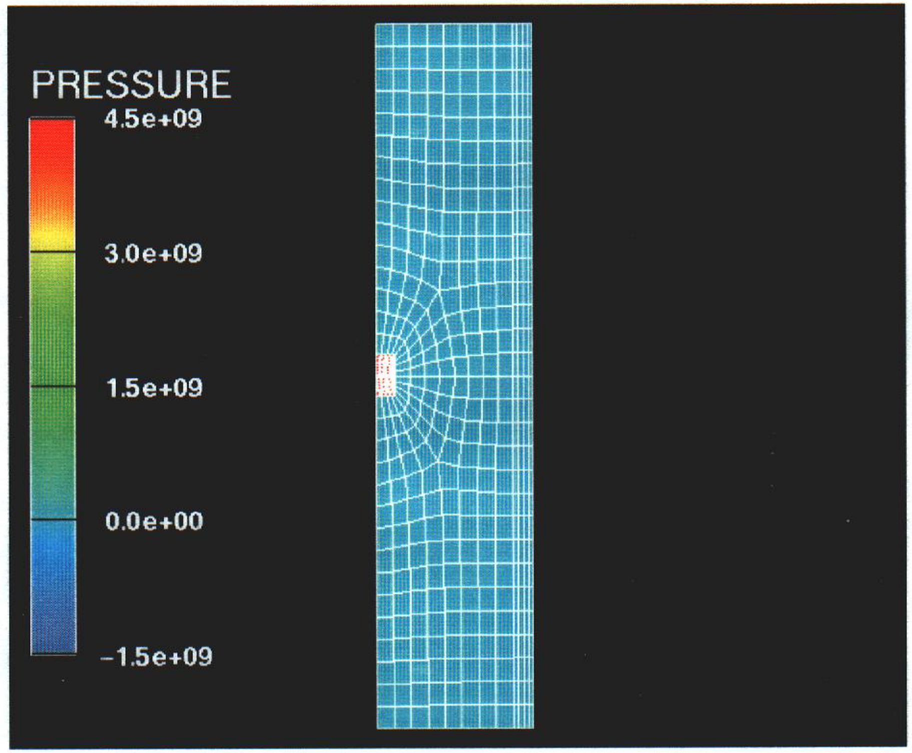
- 9" cylinder, 4" diameter, filled with water and 3-5.7g PETN explosive in center.
- Compare radial velocity and displacement.
- Demonstrate use of several methods for performing calculation:
  - Lagrangian->ALE->Eulerian for explosive and water
  - Lagrangian for cylinder
  - Initial refinement
  - H-Adaptive
  - Parallel



Sandia National Laboratories

Solid Dynamics: Hydrobulge Simulations



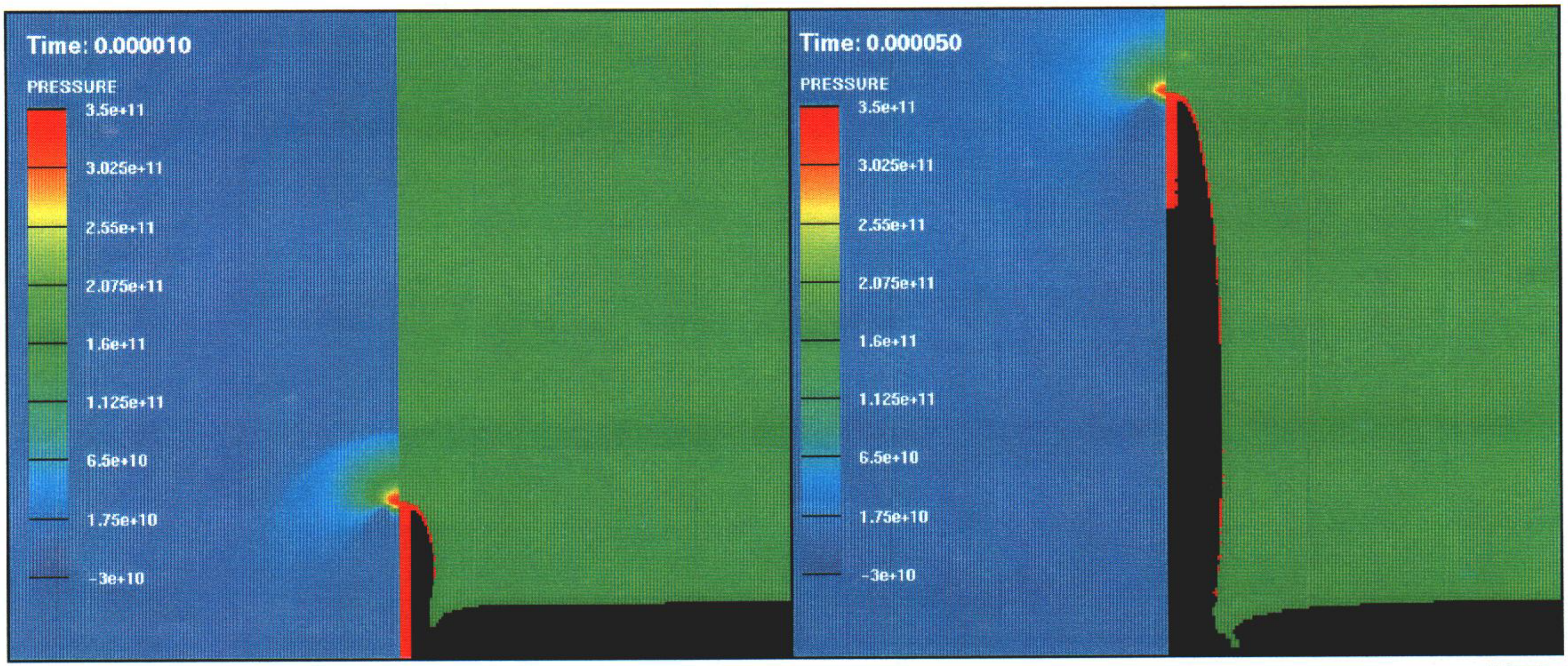


Pressure magnitude (left); with mesh overlay (right)

Sandia National Laboratories

Solid Dynamics: Long Rod Simulations

- 2D Cylindrical simulations of long tungsten rods impacting thick RHA plates
  - Impact velocities: 1 – 4.5 km/s
  - Rod Length/Mass: 12 cm / 50 gm, 15 cm / 100 gm



Sandia National Laboratories

Materials and Material Models

- Material simply defined as a collection of material models.
- Material model is an object that operates on material data.
- Elements may contain zero to all materials at any time.
- Several material models may operate in series to determine the state of the material.
- Material model may be a collection of other material models
- Provide all necessary classes of models
  - Equation of state
  - Constitutive/Yield
  - Fracture
  - HE Burn
  - Conductivity
  - Permittivity
  - and more
- Some models common with CTH and PRONTO
- Material model interface designed for modular rapid model implementation.

Sandia National Laboratories

Example Material Models

- **EOS:** Mie Gruniesen, Programmed and Reactive Burn models, SESAME
- **Constitutive:** Linear Elastic
- **Yield:** Von Mises, Johnson-Cook, Zerilli-Armstrong, Steinberg-Guinan-Lund, Sandia Visco-plastic
- **Fracture:** Pressure-based void insertion
- **Conductivity:** Lee-More
- **Structural:** Elastic-Plastic for shells

Transient Electromagnetics

Transient Electromagnetics (TEM) in ALEGRA incorporates:

- Two formulations of full-field, unstructured FETD solver with 1st order ABC (operational)
- Structured FDTD / Hybrid FETD/FDTD solver with PML (implementation in progress)
- Sub-cell algorithms for wires, slots (operational), material layers and SPICE interface (future)
- Fully coupled kinetic plasma (particles) (future)

TEM: Unconditionally Stable Helmholtz Formulation

Edge Elements (zeroth order):

$$\mathbf{w}_i^{(1)}(r) = w_{i_{n1}} \nabla w_{i_{n2}} - w_{i_{n2}} \nabla w_{i_{n1}}$$

Weak-Form of Maxwell System for Electric Field:

$$\mathbf{T}_e \frac{\partial^2}{\partial t^2} \mathbf{e}_s + \mathbf{B}_e \frac{\partial}{\partial t} \mathbf{e}_s + \mathbf{S}_e \mathbf{e}_s = -\mathbf{D}_e \frac{\partial}{\partial t} \mathbf{I}_w$$

Current Source

with

$$\mathbf{T}_e = \varepsilon_o \int dV \, \varepsilon_r \, \mathbf{w}_i^{(1)} \cdot \mathbf{w}_j^{(1)}$$ **(mass matrix)**

$$\mathbf{S}_e = \frac{1}{\mu_o} \int dV \frac{1}{\mu_r} \nabla \times \mathbf{w}_i^{(1)} \cdot \nabla \times \mathbf{w}_j^{(1)}$$

$$\mathbf{B}_e = \int dS \, \alpha \, \mathbf{n} \times \mathbf{w}_i^{(1)} \cdot \mathbf{n} \times \mathbf{w}_j^{(1)} + \int dV \, \sigma \, \mathbf{w}_i^{(1)} \cdot \mathbf{w}_j^{(1)}$$

Sandia National Laboratories

TEM: Conditionally Stable Curl-Curl Formulation

Edge and Facet Elements (zeroth order):

$$\mathbf{w}_i^{(1)}(r) = w_{i_{n1}} \nabla w_{i_{n2}} - w_{i_{n2}} \nabla w_{i_{n1}}$$

$$\mathbf{w}_i^{(2)}(r) = 2\left(w_{i_{n1}} \nabla w_{i_{n2}} \times \nabla w_{i_{n3}} + w_{i_{n2}} \nabla w_{i_{n3}} \times \nabla w_{i_{n1}} + w_{i_{n3}} \nabla w_{i_{n1}} \times \nabla w_{i_{n2}}\right)$$

Strong and Weak form Maxwell System for Magnetic and Electric Fields (respectively):

$$\frac{\partial}{\partial t}\mathbf{b}_A = -\mathbf{C}\,\mathbf{e}_s - \mathbf{D}_m\,\mathbf{V}_\mathbf{s}$$

Standard FDTD form (but on arbitrary grid)

$$\mathbf{T}_e \frac{\partial}{\partial t}\mathbf{e}_s = \mathbf{C}^t\,\mathbf{T}_f\,\mathbf{b}_A - \mathbf{D}_e\,\mathbf{I}_w$$ **with**

$$\mathbf{T}_e = \varepsilon_o \int dV\, \varepsilon_r\, \mathbf{w}_i^{(1)} \cdot \mathbf{w}_j^{(1)}$$

$$\mathbf{T}_f = \frac{1}{\mu_o} \int dV\, \frac{1}{\mu_r}\, \mathbf{w}_i^{(2)} \cdot \mathbf{w}_j^{(2)}$$

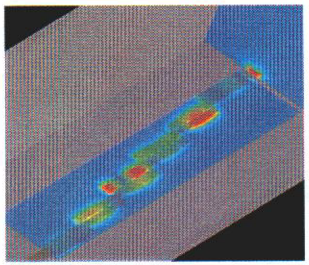
TEM: Implementation

- The TEM unstructured FETD solver inherits from Unstructured_Region
- The TEM structured FDTD solver inherits from Structured_Region
- Coupling between these regions for Hybrid EM involves a controller class
- Coupling between EM and Radiation will occur via multiple inheritance
- TEM utilizes the Aztec CG solver and Nemesis mesh decomposition

Sandia National Laboratories

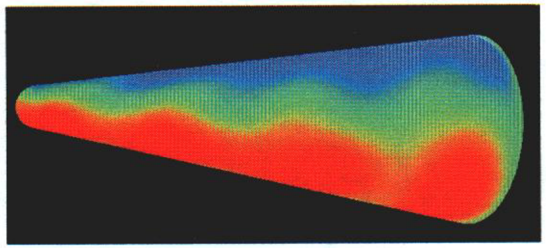
TEM: Application Areas at SNL

Electrical Packaging



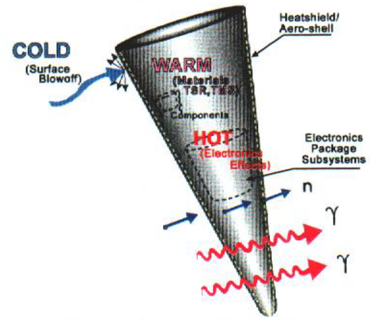
Multiple Components, Coupled EM & Non-Linear Circuits

EMR / EMC / EMI



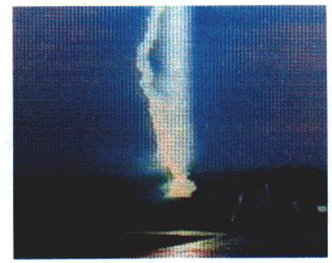
Electrically Large, Geometric Detail, High Dynamic Range

Hostile Environments



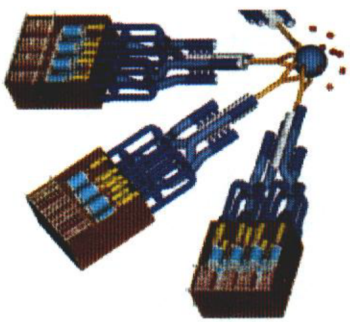
Coupled Physics, Complex Geometry

Lightning Safety



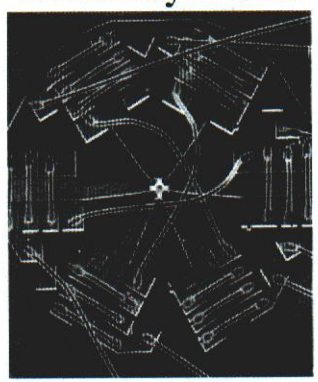
Wide Frequency Range, Complex Geometry

Beams: Radiography / Neutron Generator Tubes



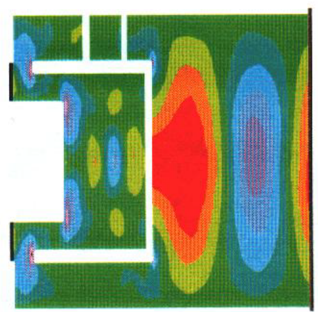
Coupled Physics, Complex Geometry

Microsystems



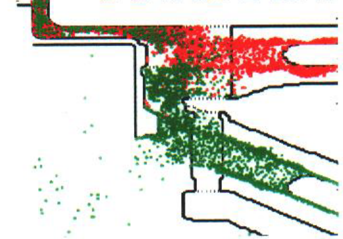
High Accuracy, Complex

Antennas / High-Power Microwaves



Large and Complex

Z-pinch Power Flow



High Magnetic Fields, Multiple Plasma Density Scales

Sandia National Laboratories

Electromechanics Overview

- **Electromechanics modeling is generally interested in time scales much larger than speed of light time scales. Maxwell equations and coupling terms can be simplified.**

$$\frac{l}{c}=\frac{0.01m}{3.0\times10^{8}m/s}=33ps=\tau_{em}>>\tau_{mechanics}$$

$$\tau_m=\mu_0\sigma_0 l^2 \qquad \tau_e=\varepsilon_0/\sigma_0$$

$\tau_m<\tau_{em}<\tau_e$ leads to electro-quasistatic mechanics

$\tau_e<\tau_{em}<\tau_m$ leads to magnetohydrodynamics

Sandia National Laboratories

Electro-quasistatic mechanics (QSEM)

- **First major coupled physics model in ALEGRA.**
- **3D perfect dielectric modeling. Coupling to external circuits through constant potential boundary conditions (perfect conductors).**
- **Modeling devices containing ferroelectric and piezoelectric materials.**
  - Piezoelectric materials produce electrical response due stress and vice-versa.
  - Ferroelectric materials exhibit piezoelectric response and a spontaneous electric polarization. Polarization and permittivity affected by the history of applied electric fields and stresses.

QSEM: Governing Equations

$$\dot{\rho} + \rho \nabla \cdot \mathbf{u} = 0$$

$$\rho \dot{\mathbf{u}} = \nabla \cdot \mathbf{T}$$

$$\rho \dot{e} = \mathbf{T} : \nabla \mathbf{u}$$

$$\nabla \cdot \mathbf{D} = 0$$

- Constitutive equations close the system.
- Example

$$\mathbf{T} = c\mathbf{S} - \hat{e}\mathbf{E}$$

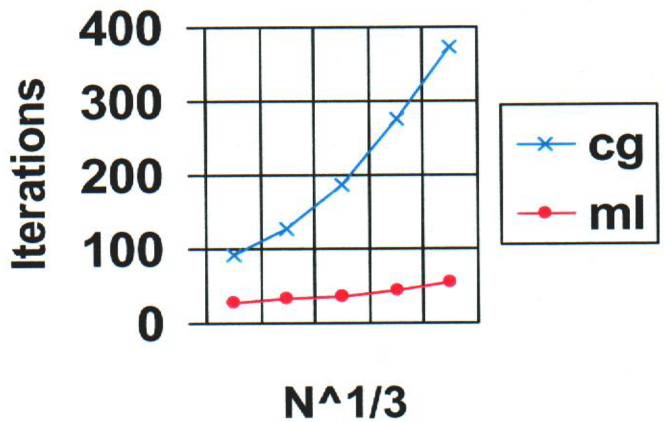
$$\mathbf{D} = \hat{e}\mathbf{S} + \varepsilon\mathbf{E}$$

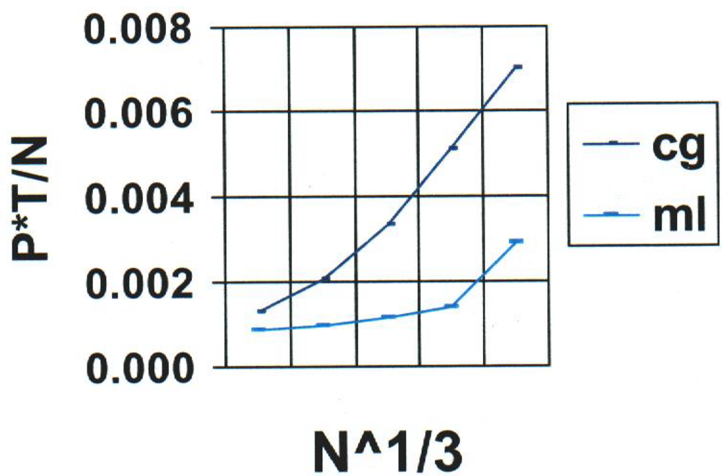
QSEM: Implementation

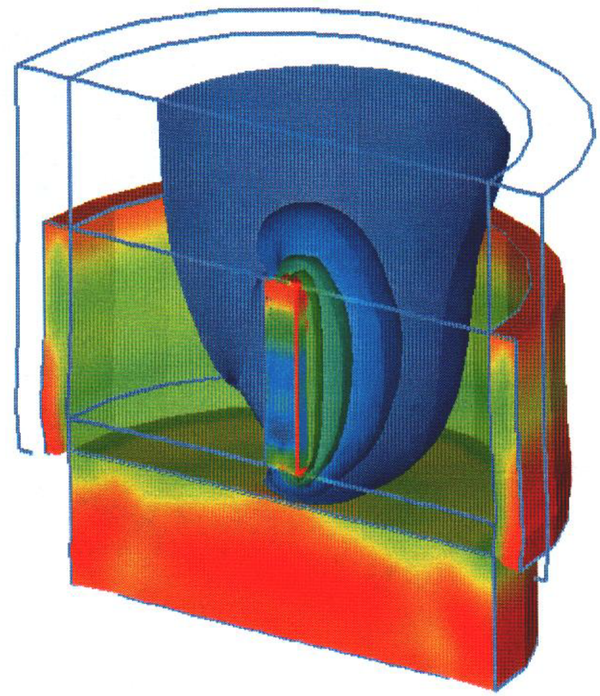
- **Electroquasistatic mechanics** $\nabla \cdot (\varepsilon \nabla \varphi) = \nabla \cdot \mathbf{p}$
  - Electroquasistatics is implemented as a separate physics class (Qse).
  - Solid dynamics is coupled with Qse through multiple inheritance and operator splitting.
  - 1 irregular hex adaptive mesh supported.
- **AZTEC/ML**
  - The Aztec/ML library solves FE matrix for electric potential.
  - Geometric multigrid using ALEGRA initial refinement capability as well as algebraic multigrid (AMG) is available.
- **DASPK** - DAE solver used to couple to external circuits.

Sandia National Laboratories

QSEM: Simulation of Ferroelectric Ceramic







Fused silica flyer plate impacting a bar of poled ceramic. Stress and electric potential isosurfaces shown.

Sandia National Laboratories

Magnetohydrodynamics (MHD)

- Magnetohydrodynamics models the motion of a fluid continuum in an electrically conducting media.
- 2D
  - Bz out of plane and Jx, Jy in the plane.
  - Btheta out of the plane Jr,Jz in the plane.
  - Jz out of the plane with Bx By in the plane (Uses vector potential Az).
- 3D
- Lagrangian/Remesh/Remap steps supported

Sandia National Laboratories

MHD: Equations

$$\dot{\rho} + \rho \nabla \cdot \mathbf{u} = 0$$

$$\rho \dot{\mathbf{u}} = \nabla \cdot \mathbf{T} + \mathbf{J} \times \mathbf{B}$$

$$\rho \dot{e} = \mathbf{T} : \nabla \mathbf{u} + \mathbf{J} \cdot \hat{\mathbf{E}}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v} + \hat{\mathbf{E}}) = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times (\mathbf{B} / \mu_0) = \mathbf{J}$$

- **Constitutive equations close the system.**

$$\mathbf{J} = \sigma(\rho, \theta) \hat{\mathbf{E}}$$

$$\mathbf{T} = -p(\rho, e) \mathbf{I}$$

- **Thermal transport and a simple emission radiation model are also available to diffuse and remove energy.**

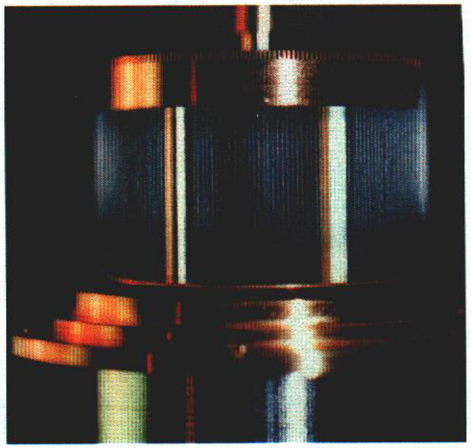
Sandia National Laboratories

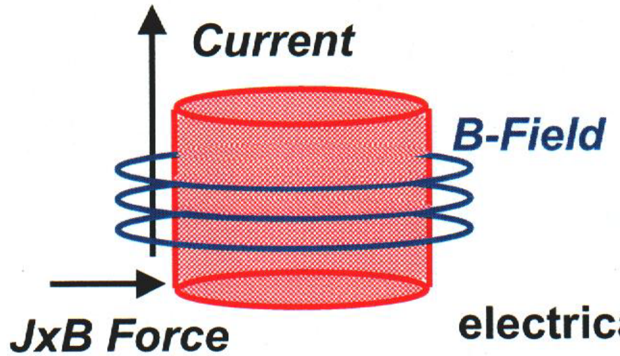
MHD: Implementation

- Transients magnetics
  - Transient magnetics is implemented as a separate physics class (Mag).
  - Solid dynamics is coupled with magnetics through multiple inheritance and operator splitting.
- AZTEC/ML
  - The Aztec library is used to solve the FE matrices.
  - A new 3D edge/face element based method currently in development requires special AMG.
  - Constrained transport magnetic flux remap strategies are under development.
- DASPK - Mesh response coupled to external circuit using DAE solver.

Sandia National Laboratories

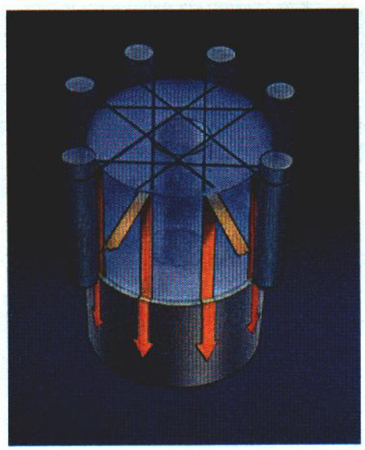
MHD: Z-pinch Applications



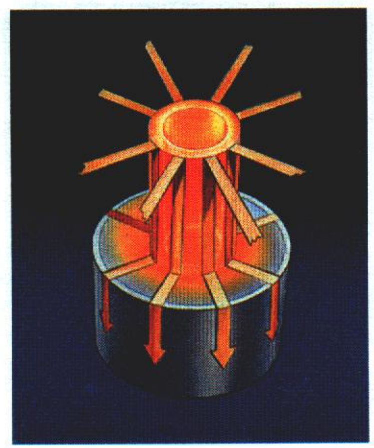


kinetic and electrical energy
↓
internal (shock heating)
↓
x rays

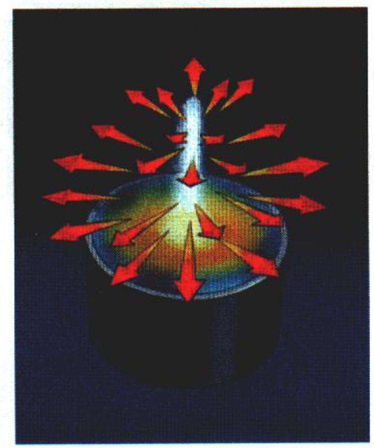
electrical energy
↓
kinetic energy



Initiation



Implosion



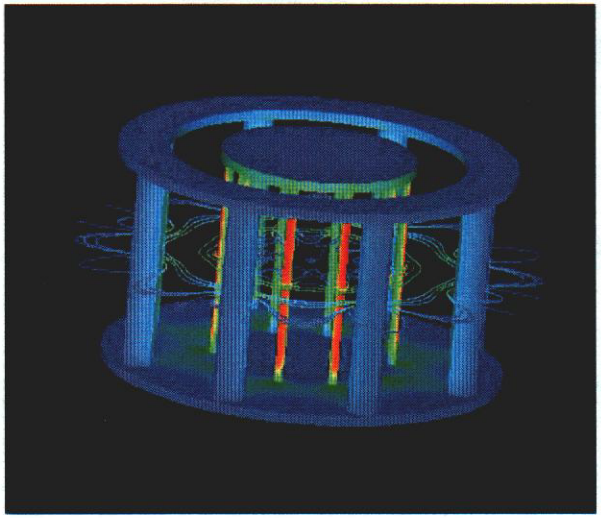
Stagnation

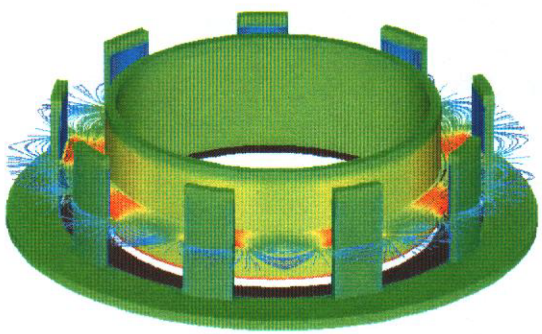
Sandia National Laboratories

MHD: Example Simulations

Transient magnetics

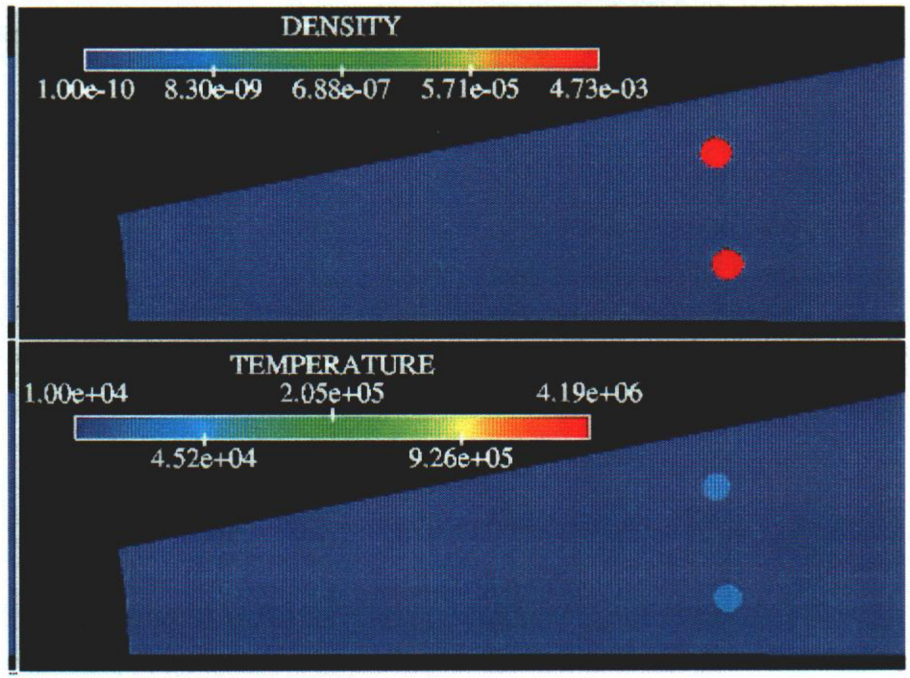
movie





Constrained transport

movie



Sandia National Laboratories

Conclusion

- ALEGRA has developed into a framework capable of integrating advanced, coupled physics using a variety of solution methods
- Examples of classes of physics solutions:
  - Solid Dynamics
  - Transient Electromagnetics
  - Electro-quasistatic mechanics
  - Magnetohydrodynamics
- Methods
  - Lagrangian, ALE, Eulerian, H-Adaptivity
  - Structured and Unstructured Meshes